

Physical Wigner functions

Carlos L. Benavides-Riveros^{1,2} and José M. Gracia-Bondía^{2,3}

¹Zentrum für Interdisziplinäre Forschung, Wellenberg 1
Bielefeld 33615, Germany

²Departamento de Física Teórica, Universidad de Zaragoza
50009 Zaragoza, Spain

³Instituto de Física Teórica, CSIC–UAM, Madrid 28049, Spain

July 30, 2012

Abstract

With an eye towards applications in chemistry, we characterize Wigner quasiprobabilities for boson-type and fermion-type wave functions or density matrices in turn. Our characterization appears to be more convenient than the one given by O’Connell and Wigner [1] some time ago.

1 Introduction

For eighty years, Wigner quasiprobability distributions (or Wigner functions for short) have been an important tool of quantum physics, successfully adopted in statistical mechanics [2], optics [3] and now quantum chemistry [4].

By definition, a pure n -body Wigner quasiprobability distribution in terms of the wave function Ψ is given by

$$\begin{aligned} W_{\Psi}(\mathbf{x}; \mathbf{p}) &:= \frac{1}{\pi^{dn}} \int \Psi(\mathbf{x} - \mathbf{z}) \Psi^*(\mathbf{x} + \mathbf{z}) e^{2i\mathbf{p} \cdot \mathbf{z}} d\mathbf{z} \\ &= \frac{1}{\pi^{dn}} \int \hat{\Psi}(\mathbf{p} - \mathbf{z}) \hat{\Psi}^*(\mathbf{p} + \mathbf{z}) e^{-2i\mathbf{x} \cdot \mathbf{z}} d\mathbf{z}, \end{aligned} \tag{1}$$

with the notation $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ for n bodies, where $\mathbf{x}_i \in \mathbb{R}^d$ (say, $d = 3$ for ordinary space), and similarly for \mathbf{p} and \mathbf{z} . Here $\hat{\Psi}$ denotes the wave function on momentum space corresponding to Ψ . We have taken units so that $\hbar = 1$.

In this context, quasiprobability means that averages of this expression with classical phase-space observables reproduce the expected values predicted by standard quantum mechanics. Wigner functions can describe statistical mixtures as well, by the usual convex linear combinations.

It is not easy to characterize Wigner functions, although necessary and sufficient conditions (not involving wave functions explicitly) for a phase-space function to be an admissible Wigner quasiprobability distribution are known [4–6].

Now, a natural question is to determine when a Wigner quasiprobability distribution does correspond to a wave function symmetric or antisymmetric under permutations of its variables. This was posed since the early days, mainly in view of applications to kinetic theory and statistical physics: see the references in [1]. But only the latter article purported to offer a general answer.¹

On their characterization, O’Connell and Wigner do write: “It must be admitted that this equation, for the distribution function, postulating the Bose statistics for a system of spin 0 particles, is much more complicated than the corresponding equation for the density matrix”. *Et pour cause*: formulas (14a) or (14b) in [1], together with formula (11) look unwieldy, so much as perhaps to have discouraged borrowing of the more interesting part of their paper [1, Sect. IV], on systems of spin $\frac{1}{2}$ particles, which unfortunately we have not seen exploited elsewhere. No examples are given.

The development of density functional theory based on Wigner quasiprobabilities [4] obliges us to revisit the matter here, from the standpoint of quantum chemistry. This means that our particles are electrons, that is, fermions; however, the orbital parts of the corresponding wave functions may be symmetric or antisymmetric. For closed-shell configurations, the spin-free part of the ground state is symmetric, while that of the first excited state is typically antisymmetric.

It should be clear that, whether Ψ is symmetric or antisymmetric, the function (1) is *symmetric* under particle interchange,

$$\begin{aligned} W_{\Psi}(\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_n; \mathbf{p}_1, \dots, \mathbf{p}_i, \dots, \mathbf{p}_j, \dots, \mathbf{p}_n) \\ = W_{\Psi}(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots, \mathbf{x}_n; \mathbf{p}_1, \dots, \mathbf{p}_j, \dots, \mathbf{p}_i, \dots, \mathbf{p}_n). \end{aligned}$$

We readily give a long-due *simple* answer to the physical indistinguishability question for W_{Ψ} . Our characterization takes the form of a mere preservation/change of sign under (the same) permutation of two variables, respectively for the symmetric/antisymmetric case —just like in the ordinary formalism of quantum mechanics. This makes it trivial that the square of a permutation induces the identity, which is not so obvious in [1]. A last bonus is that our conditions are akin to those of the general characterization problem for Wigner functions, as expounded in [4, App. B]. We illustrate them with a few example classes.

Consider first 2-body functions. Bringing in mean and difference coordinates, or, in

¹We put aside the second-quantized approach to Wigner quasiprobability, which has drawn scant attention.

chemists' jargon, *extracule* and *intracule* coordinates, respectively given by

$$\mathbf{R} = \frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{r} = \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2), \quad (2)$$

with the customary abuse of notation, the symmetry/antisymmetry conditions (say, on configuration space) $\Psi(\mathbf{x}_1, \mathbf{x}_2) = \pm \Psi(\mathbf{x}_2, \mathbf{x}_1)$ read:

$$\Psi(\mathbf{R}, \mathbf{r}) = \pm \Psi(\mathbf{R}, -\mathbf{r}).$$

It is not hard to see that with

$$\mathbf{P} = \frac{1}{\sqrt{2}}(\mathbf{p}_1 + \mathbf{p}_2), \quad \mathbf{p} = \frac{1}{\sqrt{2}}(\mathbf{p}_1 - \mathbf{p}_2), \quad (3)$$

the meaning of $W(\mathbf{R}, \mathbf{r}; \mathbf{P}, \mathbf{p})$ is unambiguous. This is due to the linear symplectic invariance of the Wigner function formalism.

If instead of the wave function we employ the density matrix $\rho(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}'_1, \mathbf{x}'_2)$, the same transformations give rise to

$$\rho(\mathbf{R}, \mathbf{r}, \mathbf{R}', \mathbf{r}') = \pm \rho(\mathbf{R}, \pm \mathbf{r}, \mathbf{R}', \mathbf{r}') = \pm \rho(\mathbf{R}, \mathbf{r}, \mathbf{R}', \pm \mathbf{r}').$$

In this case, $W_\rho(\mathbf{x}; \mathbf{p}) = \pi^{-dn} \int \rho(\mathbf{x} - \mathbf{z}; \mathbf{x} + \mathbf{z}) e^{2i\mathbf{p} \cdot \mathbf{z}} d\mathbf{z}$.

Since the discussion will turn around the intracule variables, it is worth regarding \mathbf{R}, \mathbf{P} as parameters and introducing the following notation:

$$\omega_{\mathbf{R}, \mathbf{P}}(\mathbf{r}; \mathbf{p}) := W(\mathbf{R}, \mathbf{r}; \mathbf{P}, \mathbf{p}).$$

Let us denote the following partial Fourier transform on the intracule set of variables:

$$\tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{v}; \mathbf{p}) := \int \omega_{\mathbf{R}, \mathbf{P}}(\mathbf{r}; \mathbf{p}) e^{2i\mathbf{v} \cdot \mathbf{r}} d\mathbf{r} = \tilde{\omega}_{\mathbf{R}, \mathbf{P}}(-\mathbf{v}; -\mathbf{p}).$$

The last equality holds if Ψ or ρ possesses the symmetry or the antisymmetry property.

2 When does W come from a symmetric wave function?

Proposition 1. *A Wigner two-body function comes from a boson-type density matrix if and only if, for all \mathbf{v} and \mathbf{p} :*

$$\tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{v}; \mathbf{p}) = \tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{p}; \mathbf{v}). \quad (4)$$

Proof. Consider first the following integral:

$$\begin{aligned} \tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{v}; \mathbf{p}) &= \frac{1}{\pi^{2d}} \int \Psi(\mathbf{R} - \mathbf{Z}, \mathbf{r} - \mathbf{z}) \Psi^*(\mathbf{R} + \mathbf{Z}, \mathbf{r} + \mathbf{z}) e^{2i\mathbf{P} \cdot \mathbf{Z} + 2i\mathbf{p} \cdot \mathbf{z}} e^{2i\mathbf{v} \cdot \mathbf{r}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= \frac{1}{\pi^{2d}} \int \Psi(\mathbf{R} - \mathbf{Z}, \mathbf{z} - \mathbf{r}) \Psi^*(\mathbf{R} + \mathbf{Z}, \mathbf{z} + \mathbf{r}) e^{2i\mathbf{P} \cdot \mathbf{Z} + 2i\mathbf{v} \cdot \mathbf{r}} e^{2i\mathbf{p} \cdot \mathbf{z}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= \int \omega_{\mathbf{R}, \mathbf{P}}(\mathbf{z}; \mathbf{v}) e^{2i\mathbf{p} \cdot \mathbf{z}} d\mathbf{z} = \tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{p}; \mathbf{v}). \end{aligned}$$

Conversely, retracing our steps till the second equality, one verifies that the identity (4) holds only if $\Psi \otimes \Psi^*$ defined on $\mathbb{R}^d \times \mathbb{R}^d$ is symmetric.

For the general case of statistical mixtures, exchanging the second (say) set of variables we find:

$$\begin{aligned}\tilde{\omega}_{\mathbf{R},\mathbf{P}}(\mathbf{v};\mathbf{p}) &= \frac{1}{\pi^{2d}} \int \rho(\mathbf{R} - \mathbf{Z}, \mathbf{r} - \mathbf{z}; \mathbf{R} + \mathbf{Z}, \mathbf{r} + \mathbf{z}) e^{2i\mathbf{P} \cdot \mathbf{Z} + 2i\mathbf{p} \cdot \mathbf{z}} e^{2i\mathbf{v} \cdot \mathbf{r}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= \frac{1}{\pi^{2d}} \int \rho(\mathbf{R} - \mathbf{Z}, \mathbf{z} - \mathbf{r}; \mathbf{R} + \mathbf{Z}, \mathbf{z} + \mathbf{r}) e^{2i\mathbf{P} \cdot \mathbf{Z} + 2i\mathbf{v} \cdot \mathbf{r}} e^{2i\mathbf{p} \cdot \mathbf{z}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= \tilde{\omega}_{\mathbf{R},\mathbf{P}}(\mathbf{p};\mathbf{v}).\end{aligned}$$

As before, this will hold only if ρ is symmetric. We could have argued as well from convex linear combinations of pure Wigner functions. \square

The reader may check, after a few steps, that (4) is mathematically equivalent to (14b) together with (11) in [1], when $d = 3$.

In quantum chemistry based on the Wigner function formalism [4], use of Gaussian basis sets is if anything more natural than in standard quantum chemistry [7]. This motivates the example that follows.

Example 1. Take as a boson-type wave function the symmetric product of two general Gaussians centered at the origin:

$$\Psi(x_1, x_2) = C(\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)), \quad (5)$$

where, for $j = 1, 2$:

$$\psi_j(x) = \frac{d_j^{1/4}}{\pi^{1/4}} e^{-\frac{1}{2}d_j x^2 - \frac{i}{2}b_j d_j x^2} \quad \text{with } d_j > 0, b_j \in \mathbb{R}.$$

(The normalization factor C fulfils

$$|C|^{-2} = 2 + 2\sqrt{\frac{4d_1 d_2}{(d_1 + d_2)^2 + (b_1 d_1 - b_2 d_2)^2}};$$

but this is unimportant here.) The corresponding two-body quasidensity is

$$\begin{aligned}W(x_1, x_2; p_1, p_2) &\propto W_{11}(x_1; p_1)W_{22}(x_2; p_2) + W_{22}(x_1; p_1)W_{11}(x_2; p_2) \\ &\quad + W_{12}(x_1; p_1)W_{21}(x_2; p_2) + W_{21}(x_1; p_1)W_{12}(x_2; p_2).\end{aligned} \quad (6)$$

Here W_{jk} represents an interference, namely,

$$\begin{aligned}W_{jk}(x, p) &= \frac{d_j^{1/4} d_k^{1/4}}{\pi d_{jk}^{1/2}} e^{-A_{jk} x^2 - 2B_{jk} x p - d_{jk}^{-1} p^2}, \quad \text{where} \\ d_{jk} &:= \frac{1}{2}(d_j + d_k) + \frac{i}{2}(b_j d_j - b_k d_k), \quad b_{jk} := \frac{1}{2}(b_j d_j + b_k d_k) - \frac{i}{2}(d_j - d_k), \\ A_{jk} &:= d_{jk} + b_{jk}^2/d_{jk}, \quad B_{jk} := b_{jk}/d_{jk}.\end{aligned}$$

The quadratic form in the exponent of the Gaussian is given by a symmetric, symplectic matrix with positive definite real part. When $k = j$, we have a Gaussian pure *state*,

$$W_{jj}(x, p) = \pi^{-1} e^{-(d_j + b_j^2 d_j)x^2 - 2b_j x p - d_j^{-1} p^2};$$

whose coefficient matrix is real, symplectic and positive definite [8].

To see that the quasidensity (6) fulfils (4), change variables according to (2) and (3), and let

$$\begin{aligned} \lambda_{jkkj}(R, r; P, p) &:= W_{jk}(x_1; p_1) W_{kj}(x_2; p_2) \\ &= \frac{1}{\pi^2} \sqrt{\frac{d_j d_k}{d_{jk} d_{kj}}} \exp(-A_{jk} x_1^2 - 2B_{jk} x_1 p_1 - d_{jk}^{-1} p_1^2) \exp(-A_{kj} x_2^2 - 2B_{kj} x_2 p_2 - d_{kj}^{-1} p_2^2) \\ &= \frac{1}{\pi^2} \sqrt{\frac{d_j d_k}{d_{jk} d_{kj}}} \exp[-\operatorname{Re} A_{jk}(R^2 + r^2) - 2i \operatorname{Im} A_{jk} R r - \operatorname{Re} d_{jk}^{-1}(P^2 + p^2) - 2i \operatorname{Im} d_{jk}^{-1} P p] \\ &\quad \times \exp[-2 \operatorname{Re} B_{jk}(R P + r p) - 2i \operatorname{Im} B_{jk}(r P + R p)]. \end{aligned}$$

Now, multiplying by $e^{2iv r}$ and integrating with respect to r , we obtain

$$\begin{aligned} &\frac{\sqrt{2} \pi^{-3/2}}{\sqrt{d_j + b_j^2 d_j + d_k + b_k^2 d_k}} \exp[-\operatorname{Re} A_{jk} R^2 - \operatorname{Re} d_{jk}^{-1}(P^2 + p^2) - 2i \operatorname{Im} d_{jk}^{-1} P p] \\ &\quad \times \exp[-2 \operatorname{Re} B_{jk} R P - 2i \operatorname{Im} B_{jk} R p] \exp\left[\frac{(i \operatorname{Im} A_{jk} R + \operatorname{Re} B_{jk} p + i \operatorname{Im} B_{jk} P - iv)^2}{\operatorname{Re} A_{jk}}\right]. \end{aligned}$$

We have used here that

$$d_{jk} d_{kj}(A_{jk} + A_{kj}) = d_j d_k (d_j + b_j^2 d_j + d_k + b_k^2 d_k). \quad (7)$$

Now let $W_{jj}(x_1; p_1) W_{kk}(x_2; p_2) =: \lambda_{jjkk}(R, r; P, p)$. With a little more work, using (7) again, one checks that

$$\int \lambda_{jjkk}(R, r; P, p) e^{2iv r} dr = \int \lambda_{jkkj}(R, r; P, v) e^{2ip r} dr \quad \text{with } k \neq j,$$

thereby verifying condition (4) for this example.

3 When does W come from an antisymmetric wave function?

Proposition 2. *A Wigner two-body function comes from a fermion-type density matrix if and only if, for all \mathbf{v} and \mathbf{p} :*

$$\tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{v}; \mathbf{p}) = -\tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{p}; \mathbf{v}). \quad (8)$$

Proof. We argue from wave functions. As in the boson-type case, we consider the following integral:

$$\begin{aligned}\tilde{\omega}_{\mathbf{R},\mathbf{P}}(\mathbf{v};\mathbf{p}) &= \frac{1}{\pi^{2d}} \int \Psi(\mathbf{R}-\mathbf{Z},\mathbf{r}-\mathbf{z}) \Psi^*(\mathbf{R}+\mathbf{Z},\mathbf{r}+\mathbf{z}) e^{2i\mathbf{P}\cdot\mathbf{Z}+2i\mathbf{p}\cdot\mathbf{z}} e^{2i\mathbf{v}\cdot\mathbf{r}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= -\frac{1}{\pi^{2d}} \int \Psi(\mathbf{R}-\mathbf{Z},\mathbf{z}-\mathbf{r}) \Psi^*(\mathbf{R}+\mathbf{Z},\mathbf{z}+\mathbf{r}) e^{2i\mathbf{P}\cdot\mathbf{Z}+2i\mathbf{v}\cdot\mathbf{r}} e^{2i\mathbf{p}\cdot\mathbf{z}} d\mathbf{r} d\mathbf{Z} d\mathbf{z} \\ &= -\int \omega_{\mathbf{R},\mathbf{P}}(\mathbf{z};\mathbf{v}) e^{2i\mathbf{p}\cdot\mathbf{z}} d\mathbf{z} = -\tilde{\omega}_{\mathbf{R},\mathbf{P}}(\mathbf{p};\mathbf{v}).\end{aligned}$$

Therefore (8) holds if and only if $\Psi \otimes \Psi^*$ defined on $\mathbb{R}^d \times \mathbb{R}^d$ is antisymmetric. \square

As a consequence of formula (8), a *necessary* condition for a Wigner function to come from an antisymmetric wave function is $\tilde{\omega}_{\mathbf{R},\mathbf{P}}(\mathbf{p};\mathbf{p}) = 0$. This is not sufficient, since any one-dimensional wave function (say) of the form $\Psi(R,r) = f(R)g(r)$ with $\int g(r) dr = 0$ will give rise to a Wigner function having that property.

As for examples, it is clear that Gaussian sets like the ones in (5) with a minus instead of a plus sign will do. However, it is more instructive now to take a different tack. In the early years of Quantum Mechanics, as a prolegomenon to calculating the energy levels for helium, Heisenberg [9] studied the *harmonium*, an exactly integrable analogue of a two-electron atom. It exhibits two fermions interacting with an external harmonic potential and repelling each other by a Hooke-type force. Being simple, but not trivial, this system has been borrowed in many contexts. It is sometimes called the “Moshinsky atom”, since Moshinsky reintroduced it with the purpose of studying correlation energy [10,11]. Also, it has been employed in approaches to Bose–Einstein condensation [12] and black-hole entropy [13].

The harmonium Hamiltonian in Hartree-like units is given by:

$$H(\mathbf{x}_1, \mathbf{x}_2; \mathbf{p}_1, \mathbf{p}_2) = \frac{|\mathbf{p}_1|^2}{2} + \frac{|\mathbf{p}_2|^2}{2} + \frac{k}{2}(|\mathbf{x}_1|^2 + |\mathbf{x}_2|^2) - \frac{\delta}{4}|\mathbf{x}_1 - \mathbf{x}_2|^2.$$

Introducing extracule and intracule coordinates and the frequencies $\nu := \sqrt{k}$ and $\mu := \sqrt{k - \delta}$, the Hamiltonian is rewritten as that of two independent oscillators:

$$H = H_R + H_r := \frac{|\mathbf{P}|^2}{2} + \frac{\nu^2|\mathbf{R}|^2}{2} + \frac{|\mathbf{p}|^2}{2} + \frac{\mu^2|\mathbf{r}|^2}{2}.$$

Example 2. Since the harmonium problem factorizes completely, we may work in dimension one. The *orbital* part of such an eigenfunction is written $\phi_n(R)\psi_m(r)$, where the parity of $\psi_m(r)$ must be even for spin singlet states and odd for triplet states. The Wigner quasiprobabilities associated to those eigenvectors have the general form: $W_n(R, P)W_m(r, p)$, where, with L_n denoting the n -th Laguerre polynomial [14,15]:

$$\begin{aligned}W_n(R, P) &= \frac{(-1)^n}{\pi} L_n(4H_R/\nu) e^{-2H_R/\nu}, \\ W_m(r, p) &= \frac{(-1)^m}{\pi} L_m(4H_r/\mu) e^{-2H_r/\mu}.\end{aligned}$$

The generating function of the Laguerre polynomials is:

$$(1-x)^{-1} e^{-tx/(1-x)} = \sum_{m=0}^{\infty} L_m(t) x^m.$$

Defining

$$\Gamma_m(v, p) = (-1)^m \int W_m(r, p) e^{2ivr} dr = \frac{1}{\pi} \int L_m(4H_r/\mu) e^{-2H_r/\mu} e^{2ivr} dr,$$

we obtain

$$\begin{aligned} \sum_{m=0}^{\infty} \Gamma_m(v, p) x^m &= \frac{1}{\pi(1-x)} \int e^{-4(H_r/\mu)x/(1-x)} e^{-2(H_r/\mu)} e^{2ivr} dr \\ &= \frac{1}{\pi(1-x)} e^{-\frac{1+x}{1-x} p^2/\mu} \int e^{-\frac{1+x}{1-x} \mu r^2 + 2ivr} dr \\ &= \frac{1}{\sqrt{\pi\mu(1-x^2)}} \exp\left(-\frac{1+x}{1-x} \frac{p^2}{\mu} - \frac{1-x}{1+x} \frac{v^2}{\mu}\right) = \sum_{m=0}^{\infty} (-1)^m \Gamma_m(p, v) x^m. \end{aligned}$$

Thus, $\Gamma_m(v, p) = -\Gamma_m(p, v)$ if m is odd and $\Gamma_m(v, p) = \Gamma_m(p, v)$ if m is even. In particular, whenever the function $\Psi_{nm} \equiv \phi_n \psi_m$ is antisymmetric, the corresponding Wigner function $W_{nm}(R, P; r, p) = W_n(R, P) W_m(r, p)$ in agreement with (8) must satisfy:

$$\int W_{nm}(R, P; r, p) e^{2ivr} dr = - \int W_{nm}(R, P; r, v) e^{2ipr} dr.$$

Needless to say, we could have formulated our conclusions in a completely analogous manner in terms of $\hat{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{r}, \mathbf{s}) := \int \omega_{\mathbf{R}, \mathbf{P}}(\mathbf{r}; \mathbf{p}) e^{-2i\mathbf{s} \cdot \mathbf{p}} d\mathbf{p}$ instead of $\tilde{\omega}_{\mathbf{R}, \mathbf{P}}(\mathbf{v}; \mathbf{p})$.

4 The general n -body case

Our results here easily extend to n -body systems just by considering intracule and extracule coordinates for each pair of particles. This gives rise to $n(n-1)/2$ conditions like the ones above. The details are obvious, and we omit them.

Acknowledgments

We are most grateful to Joseph C. Várilly for a careful reading of the manuscript. CLBR has been supported by a Banco Santander scholarship. JMGB has been supported by a grant from the regional government of Aragón. He owes as well to the Zentrum für interdisziplinäre Forschung, for support and warm hospitality.

References

- [1] R. F. O’Connell and E. P. Wigner, Phys. Rev. A **30** 2613 (1984).
- [2] E. P. Wigner, Phys. Rev. **40** 749 (1932).
- [3] U. Leonhardt, *Essential Quantum Optics*, Cambridge University Press, Cambridge, 2010.
- [4] Ph. Blanchard, J. M. Gracia-Bondía and J. C. Várilly, Int. J. Quant. Chem. **112** 1134 (2012).
- [5] F. J. Narcowich and R. F. O’Connell, Phys. Rev. A **34** 1 (1986).
- [6] J. M. Gracia-Bondía and J. C. Várilly, Phys. Lett. A **128** 20 (1988).
- [7] F. Jensen, *Introduction to Computational Chemistry*, Wiley, Chichester, 2007.
- [8] R. G. Littlejohn, Phys. Rep. **138** 193 (1986).
- [9] W. Heisenberg, Z. Physik **38** 411 (1926).
- [10] M. Moshinsky, Am. J. Phys. **36** 52 (1968).
- [11] K. Ebrahimi-Fard and J. M. Gracia-Bondía, J. Math. Chem. **50** 440 (2012).
- [12] R. Seiringer, Ph. D. thesis, Vienna, 2000.
- [13] M. Srednicki, Phys. Rev. Lett. **71** 666 (1993).
- [14] C. L. Benavides-Riveros, J. M. Gracia-Bondía and J. C. Várilly, “The lowest excited configuration of harmonium”, physics.chem-ph/1205.2038.
- [15] C. L. Benavides-Riveros and J. C. Várilly, “Testing one-body density functionals on a solvable model”, physics.chem-ph/1207.3897.